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TERMINAL (ENTER 1, 2, 3, OR ?):2

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| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | | "Ask CAS" for self-help around the-clock |
| NEWS 3 | Jul 12 | BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS |
| NEWS 4 | Jul 30 | BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting |
| NEWS 5 | AUG 02 | IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields |
| NEWS 6 | AUG 02 | CAplus and CA patent records enhanced with European and Japan Patent Office Classifications |
| NEWS 7 | AUG 02 | The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available |
| NEWS 8 | AUG 04 | Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004 |
| NEWS 9 | AUG 27 | BIOCOMMERCE: Changes and enhancements to content coverage |
| NEWS 10 | AUG 27 | BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC |
| NEWS 11 | SEP 01 | INPADOC: New family current-awareness alert (SDI) available |
| NEWS 12 | SEP 01 | New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! |
| NEWS 13 | SEP 01 | New display format, HITSTR, available in WPIDS/WPINDEX/WPIX |
| NEWS 14 | SEP 14 | STN Patent Forum to be held October 13, 2004, in Iselin, NJ |

| | |
|---|---|
| NEWS EXPRESS | JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

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FILE 'HOME' ENTERED AT 13:59:23 ON 23 SEP 2004

=> file registry

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 13:59:44 ON 23 SEP 2004


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 SEP 2004 HIGHEST RN 749824-02-0
DICTIONARY FILE UPDATES: 22 SEP 2004 HIGHEST RN 749824-02-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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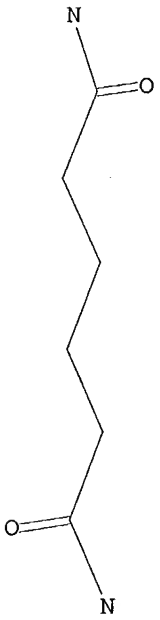
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10075017\10075017B.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR




Structure attributes must be viewed using STN Express query preparation.

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=> s l1 full
FULL SEARCH INITIATED 14:00:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 475941 TO ITERATE

 84.0% PROCESSED  400000 ITERATIONS                          4796 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.08

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       475941 TO   475941
PROJECTED ANSWERS:            5480 TO     5932

L2          4796 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.84     156.05

FILE 'CAPLUS' ENTERED AT 14:00:48 ON 23 SEP 2004
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FILE COVERS 1907 - 23 Sep 2004  VOL 141 ISS 13
FILE LAST UPDATED: 22 Sep 2004  (20040922/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2 and ligand and (channel or pump or transport or transporter)
          1550 L2
        264845 LIGAND
        229188 CHANNEL
        106220 PUMP
        625070 TRANSPORT
         33509 TRANSPORTER
L3           2 L2 AND LIGAND AND (CHANNEL OR PUMP OR TRANSPORT OR TRANSPORTER)

=> t ti l3 1-2

L3   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Interaction between iron(II) and hydroxamic acids: oxidation of iron(II)
     to iron(III) by desferrioxamine B under anaerobic conditions

L3   ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Nanoparticles containing an active agent and a poly(tartaramide ketal)
```

=> d ibib abs l3 1-2

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:94960 CAPLUS
DOCUMENT NUMBER: 134:337180
TITLE: Interaction between iron(II) and hydroxamic acids: oxidation of iron(II) to iron(III) by desferrioxamine B under anaerobic conditions
AUTHOR(S): Farkas, E.; Enyedy, E. A.; Zekany, L.; Deak, G.
CORPORATE SOURCE: Department of Inorganic and Analytical Chemistry, University of Debrecen, Debrecen, H-4010, Hung.
SOURCE: Journal of Inorganic Biochemistry (2001), 83(2-3), 107-114
CODEN: JIBIDJ; ISSN: 0162-0134
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Interaction between iron(II) and acetohydroxamic acid (Aha), α-alaninehydroxamic acid (α-Alaha), β-alaninehydroxamic acid (β-Alaha), hexanedioic acid bis(3-hydroxycarbamoyl-methyl)amide (Dha) or desferrioxamine B (DFB) under anaerobic conditions was studied by pH-metric and UV-Visible spectrophotometric methods. The stability consts. of complexes formed with Aha, α-Alaha, β-Alaha and Dha were calculated and turned out to be much lower than those of the corresponding iron(III) complexes. Stability consts. of the iron(II)-hydroxamate complexes are compared with those of other divalent 3d-block metal ions and the Irving-Williams series of stabilities was found to be observed Above pH 4, in the reactions between iron(II) and desferrioxamine B, the oxidation of the metal ion to iron(III) by the **ligand** was found. The overall reaction that resulted in the formation of the tris-hydroxamato complex [Fe(HDFB)]+ and monoamide derivative of DFB at pH 6 is:2Fe2++3H4DFB+=2[Fe(HDFB)]++H3DFB-monoamide++H2O+4H+. Based on these results, the conclusion is that desferrioxamine B can uptake iron in iron(III) form under anaerobic conditions.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:851985 CAPLUS
DOCUMENT NUMBER: 124:185539
TITLE: Nanoparticles containing an active agent and a poly(tartaramide ketal)
INVENTOR(S): Ahlers, Michael; Walch, Axel; Seipke, Gerhard; Russell-Jones, Gregory
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 671169 | A1 | 19950913 | EP 1995-103045 | 19950303 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| DE 4407898 | A1 | 19950914 | DE 1994-4407898 | 19940309 |
| TW 457096 | B | 20011001 | TW 1995-84101519 | 19950220 |
| FI 9501053 | A | 19950910 | FI 1995-1053 | 19950307 |
| US 5674531 | A | 19971007 | US 1995-399474 | 19950307 |
| IL 112905 | A1 | 20000831 | IL 1995-112905 | 19950307 |

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|---|---|---|---|---|---|
| CA 2144216 | AA | 19950910 | CA 1995-2144216 | | 19950308 |
| NO 9500889 | A | 19950911 | NO 1995-889 | | 19950308 |
| AU 9514701 | A1 | 19950921 | AU 1995-14701 | | 19950308 |
| AU 685577 | B2 | 19980122 | | | |
| JP 07258114 | A2 | 19951009 | JP 1995-48006 | | 19950308 |
| ZA 9501910 | A | 19951113 | ZA 1995-1910 | | 19950308 |
| HU 72033 | A2 | 19960328 | HU 1995-698 | | 19950308 |
| PRIORITY APPLN. INFO.: | | | DE 1994-4407898 | A | 19940309 |

GI For diagram(s), see printed CA Issue.

AB Nanoparticles of poly(tartaramide ketal) [I; R2 = (substituted) alkylene, cycloalkylene] are useful as biocompatible, biodegradable carriers for drugs, especially peptides and proteins. The nanoparticles may be functionalized with specific ligands which facilitate receptor-mediated **transport** through the intestinal wall. Thus, DL-tartaric acid was refluxed in MeOH with 2,2-dimethoxypropane and p-toluenesulfonic acid to form di-Me 2,3-O-isopropylidene-DL-tartrate, which was polymerized with 1,8-diaminooctane. A solution of this polymer 280, polylysine 60, and insulin 40 mg in MeOH was spray dried to produce nanoparticles 330 nm in diameter

=> FIL STNGUIDE

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 16.58 | 172.63 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -1.40 | -1.40 |

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LAST RELOADED: Sep 17, 2004 (20040917/UP).

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.36 | 172.99 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -1.40 |

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FILE COVERS 1907 - 23 Sep 2004  VOL 141 ISS 13
FILE LAST UPDATED: 22 Sep 2004  (20040922/ED)

  This file contains CAS Registry Numbers for easy and accurate
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     (FILE 'HOME' ENTERED AT 13:59:23 ON 23 SEP 2004)

     FILE 'REGISTRY' ENTERED AT 13:59:44 ON 23 SEP 2004
L1             STRUCTURE UPLOADED
L2          4796 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 14:00:48 ON 23 SEP 2004
L3             2 S L2 AND LIGAND AND (CHANNEL OR PUMP OR TRANSPORT OR TRANSPORTE

     FILE 'STNGUIDE' ENTERED AT 14:03:12 ON 23 SEP 2004

     FILE 'CAPLUS' ENTERED AT 14:06:39 ON 23 SEP 2004

=> s l2 and ligand
          1550 L2
        264845 LIGAND
L4           49 L2 AND LIGAND

=> t ti l4 1-49

L4   ANSWER 1 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Orthogonal Control of Dissociation Dynamics Relative to Thermodynamics in
     a Main-Chain Reversible Polymer

L4   ANSWER 2 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Preparation of novel chiral samarium(II) complexes and their application
     to asymmetric synthesis

L4   ANSWER 3 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   C2-symmetric inhibitors of Plasmodium falciparum plasmepsin II: synthesis
     and theoretical predictions

L4   ANSWER 4 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Potentiating vanadium-evoked glucose metabolism by novel hydroxamate
     derivatives

L4   ANSWER 5 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Ruthenium complexes for organic electrochromic materials for optical
     attenuation in the near infrared region

L4   ANSWER 6 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Pyrrolidine derivatives for depletion of an unwanted protein population
     from plasma

L4   ANSWER 7 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Method of identifying inhibitors of Cdc25 using three dimensional crystal
     structure of the catalytic domain of Cdc25

L4   ANSWER 8 OF 49  CAPLUS  COPYRIGHT 2004 ACS on STN
TI   Crystal structure and three-dimensional structure of human Cdc25 catalytic
     domains and its use in designing peptidomimetic inhibitors

L4 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI In vivo imaging of human colon cancer xenografts in immunodeficient mice using a guanylyl cyclase C-specific **ligand**

L4 ANSWER 10 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI IR and Raman spectra of lanthanide nitrate complexes with TBAA

L4 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Half-sandwich ruthenium(II) compounds comprising heteroatom containing ligands for treatment of cancer

L4 ANSWER 12 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Erythropoietin Mimetics Derived from Solution Phase Combinatorial Libraries

L4 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Syntheses and structures of two mixed ligands lanthanide complexes with N,N'-substituted adipamide

L4 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI A structure-function study of **ligand** recognition by CD22β

L4 ANSWER 15 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Crystal structure of CDC25 proteins and its use in rational design of inhibitors

L4 ANSWER 16 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Interaction between iron(II) and hydroxamic acids: oxidation of iron(II) to iron(III) by desferrioxamine B under anaerobic conditions

L4 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis, Crystal Structure, Spectral Studies, and Catechol Oxidase Activity of Trigonal Bipyramidal Cu(II) Complexes Derived from a Tetradentate Diamide Bisbenzimidazole **Ligand**

L4 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis, electrochemistry, and photophysics of a novel binuclear polypyridyl Ru(II) complex with an 1,8-adipoylamidobis(1,10-phenanthroline-5-yl) **ligand**

L4 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Developing carrier complexes for "caged NO": RuCl3(NO)(H2O)2 complexes of dipyridylamine, (dpaH), N,N,N'N'-tetrakis(2-pyridyl)adipamide, (tpada), and (2-pyridylmethyl)iminodiacetate, (pida2-)

L4 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Estimation of Receptor-**Ligand** Interactions by the Use of a Two-Marker System in Affinity Capillary Electrophoresis

L4 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI [RuII(hedta)]- complexes of 2,2'-dipyridylamine (dpaH) and a bifunctional tethered analog, N,N,N',N'-tetrakis(2-pyridyl)adipamide (tpada)

L4 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI A surface-modified functional liposome capable of binding to cell membranes

L4 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis of a novel lipopeptide with α-melanocyte-stimulating hormone peptide **ligand** and its effect on liposome stability. [Erratum to document cited in CA131:88183]

L4 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Preparation of N-(4-amino-6-quinolyl)carboxamides as chemokine receptor ligands and as anti-AIDS drugs

L4 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Binding of a dimeric derivative of vancomycin to L-Lys-D-Ala-D-lactate in solution and at a surface

L4 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis of a novel lipopeptide with α-melanocyte-stimulating hormone peptide **ligand** and its effect on liposome stability

L4 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis and characterization of model compounds of the active site of the enzyme superoxide dismutase

L4 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis of neoglycoconjugate dendrimers

L4 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Cytotoxicity of (2,2':6',2''-Terpyridine)platinum(II) Complexes to Leishmania donovani, Trypanosoma cruzi, and Trypanosoma brucei

L4 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Interaction between Mo(VI) and siderophore models in aqueous solution

L4 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI The use of affinity capillary electrophoresis for determining binding constants of ligands to receptors

L4 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Modification of receptor selectivity and functional activity of cyclic cholecystokinin analogs

L4 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Platinum(IV) complexes of vicinal-1,2-diamines and bis(vicinal-1,2-diamines) with an acylamino function. Evidence for a platinum hydroperoxide intermediate upon oxidation

L4 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Bis[4'-(4-anilino)-2,2':6',2"-terpyridine]transition-metal complexes: electrochemically active monomers with a range of magnetic and optical properties for assembly of metallo oligomers and macromolecules

L4 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Behavior of Ruthenium Trisbipyridine-Anthraquinone Conjugates Connected with Alkyl Spacers in Homogeneous and Microheterogeneous Media

L4 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Molecular Interaction of DNA with Bisplatinum(II) Complexes Having Bis(Vicinal 1,2-Diamines) as **Ligand**

L4 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Preparation of terpyridine-platinum(II) complexes as potent intercalators of DNA, and as antitumor and antiparasitic agents

L4 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI dl-Selective reductive coupling/Dieckmann condensation sequence of α,β-unsaturated amides with samarium(II) iodide/HMPA. Synthesis of a new **ligand**, trans-1,2-cyclopentanediyl-2,2'-bis(phenol)

L4 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

TI Preparation and characterization of mixed-**ligand** dihydrazone complexes of nickel(II)

L4 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Nanoparticles containing an active agent and a poly(tartaramide ketal)

L4 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis, characterization and biological activity of metal complexes of N,N'-bis(8-hydroxy-5-quinolinyl)adipamide

L4 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis and structure of μ-tetrabutyladipamide lanthanum(III) binuclear complex La2μ-[Bu2NCO(CH2)4CONBu2][Bu2NCO(CH2)4CONBu2]2(NO3)6

L4 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis, properties and structure of some lanthanide nitrate binuclear complex with N,N,N',N'-tetrabutyladipamide [Ln2μ-{Bu2NCO(CH2)4CONBu2}{Bu2NCO(CH2)4CONBu2}2(NO3)6]

L4 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Determination of Binding Constants of Ligands to Proteins by Affinity Capillary Electrophoresis: Compensation for Electroosmotic Flow

L4 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis and opioid receptor affinity of bivalent ligands derived from 3,8-diazabicyclo(3.2.1)octanes

L4 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Use of affinity capillary electrophoresis to determine kinetic and equilibrium constants for binding of arylsulfonamides to bovine carbonic anhydrase

L4 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Use of affinity capillary electrophoresis to measure binding constants of ligands to proteins

L4 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Synthesis and pharmacological evaluation of the anticonvulsant activity of bivalent ligands derived from 4-amino-2',6'-dimethylbenzanilide

L4 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
TI Molecular recognition between oligopeptides and nucleic acids: DNA binding specificity of a series of bis netropsin analogs deduced from footprinting analysis

=> d ibib abs l4, 3,4,7,8,9,11,12-15,20-29,31,32,37,38,40,41,44,45,47-49

L4 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:595171 CAPLUS
DOCUMENT NUMBER: 140:159483
TITLE: C2-symmetric inhibitors of Plasmodium falciparum plasmepsin II: synthesis and theoretical predictions
AUTHOR(S): Ersmark, Karolina; Feierberg, Isabella; Bjelic, Sinisa; Hulten, Johan; Samuelsson, Bertil; Aqvist, Johan; Hallberg, Anders
CORPORATE SOURCE: BMC, Department of Medicinal Chemistry, Uppsala University, Uppsala, SE-751 23, Swed.
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(17), 3723-3733
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of C2-sym. compds. with a mannitol-based scaffold has been investigated, both theor. and exptl., as Plm II inhibitors. Four different stereoisomers with either benzyloxy or allyloxy P1/P1' side chains were studied. Computational ranking of the binding affinities of the eight compds. was carried out using the linear interaction energy (LIE) method relying on a complex previously determined by crystallog. Within both series of isomers the theor. binding energies were in agreement with the enzymic measurements, illustrating the power of the LIE method for the prediction of **ligand** affinities prior to synthesis. The structural models of the enzyme-inhibitor complexes obtained from the MD simulations provided a basis for interpretation of further structure-activity relationships. Hence, the affinity of a structurally similar **ligand**, but with a different P2/P2' substituent was examined using the same procedure. The predicted improvement in binding constant agreed well with exptl. results.
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:521636 CAPLUS
DOCUMENT NUMBER: 140:157168
TITLE: Potentiating vanadium-evoked glucose metabolism by novel hydroxamate derivatives
AUTHOR(S): Hindi, Sagit; Grossman, Dov P.; Goldwaser, Itzhak; Shechter, Yoram; Fridkin, Mati
CORPORATE SOURCE: Department of Organic Chemistry, The Weizmann Institute of Science, Rehovot, Israel
SOURCE: Letters in Peptide Science (2003), Volume Date 2002, 9(6), 235-254
CODEN: LPSCEM; ISSN: 0929-5666
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB L-Glutamic acid (γ) monohydroxamate (L-Glu(γ)HXM) enhances the insulinomimetic activity of vanadium ions both in vitro and in vivo. Based on this **ligand** as a lead compound, and in order to delineate mol. features relevant to its anti-diabetic potential, 14 related derivs., including short peptides, were synthesized by solution as well as by solid phase methodologies. In addition, hydroxamate derivs. of (+) pantothenic acid and D-biotin were prepared The vanadium binding capacity of the hydroxamates synthesized was apparent, yet each had a different **ligand**-ions stoichiometry. The in vitro lipogenic potency of several compds. toward rat adipocytes was demonstrated. Thus, vanadium complexes of L-Gln(α)HXM, L-Glu(γ)HXM-Gly, L-Aad(δ)HXM, di-Glu-γ,γ-HXM and of (+) pantothenic acid hydroxamate exhibited 82, 79, 76, 39 and 39% of maximal insulin activity, resp. L-Aad(δ)HXM, L-Glu(γ)HXM-Gly and (+) pantothenic acid hydroxamate - by themselves - were found to possess 24, 14 and 10% of maximal insulin activity, resp. In vivo potency, however, of L-Gln(α)HXM vanadium complex in streptozocin-treated rat diabetic model was less apparent.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:928230 CAPLUS
DOCUMENT NUMBER: 138:19472
TITLE: Method of identifying inhibitors of Cdc25 using three dimensional crystal structure of the catalytic domain of Cdc25

INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): Australia
SOURCE: U.S. Pat. Appl. Publ., 246 pp., Cont.-in-part of U.S. Ser. No. 645,750.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| US 2002183249 | A1 | 20021205 | US 2001-797500 | | 20010301 |
| PRIORITY APPLN. INFO.: | | | US 1999-172215P | P | 19990831 |
| | | | US 2000-645750 | A2 | 20000824 |

OTHER SOURCE(S): MARPAT 138:19472
AB The present invention relates to the x-ray crystallog. study of proteins comprising the catalytic domains of Cdc25. The atomic coordinates which result from this study are of use in identifying compds. which fit in the catalytic domain and are, therefore, potential inhibitors of Cdc25. The present invention further provides proteins which comprise the **ligand** binding domain of Cdc25, crystalline forms of these proteins and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Cdc25. The invention also relates to the use of the three dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. These Cdc25 inhibitors are of use in methods of treating a patient having a condition which is modulated by Cdc25 activity, for example, a condition characterized by excessive, inappropriate or undesirable cellular proliferation such as cancer.

L4 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:696111 CAPLUS
DOCUMENT NUMBER: 137:228607
TITLE: Crystal structure and three-dimensional structure of human Cdc25 catalytic domains and its use in designing peptidomimetic inhibitors
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany; GPC Biotech Inc.
SOURCE: PCT Int. Appl., 351 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002070680 | A1 | 20020912 | WO 2001-US6587 | 20010301 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, | | | | |

CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: WO 2001-US6587 20010301

OTHER SOURCE(S): MARPAT 137:228607

AB Due to its role in regulating the cell cycle, Cdc25 (a family of dual specificity phosphatases) is a potential target for therapies aimed at controlling proliferative diseases, but rational, structure-based design has not been possible because of the lack of accurate 3-dimensional data. The present invention relates to polypeptides which comprises the **ligand** binding domain of human Cdc25 proteins, crystalline forms of these polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of Cdc25. In particular, a high resolution crystal structure was obtained for the polypeptide denoted CDC25B(ΔN8B), comprising residues Glu-368 through Arg-562 of human Cdc25B, complexed with a pentapeptide inhibitor denoted cdc1249 (2-methoxynaphthyl-1-carboxy-(4-sulfomethyl)-L-Phe-L-Glu-L-Glu-L-naphthylalanine-L-Glu-amide). The invention also relates to the use of the 3-dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. The syntheses and structures of a large number of putative pentapeptide inhibitors are also provided. Such inhibitors have potential in the treatment of diseases associated with excessive cellular proliferation, such as cancer, restenosis, reocclusion of coronary artery, and inflammation.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:386498 CAPLUS

DOCUMENT NUMBER: 138:52011

TITLE: In vivo imaging of human colon cancer xenografts in immunodeficient mice using a guanylyl cyclase C-specific **ligand**

AUTHOR(S): Wolfe, Henry R.; Mendizabal, Marivi; Lleong, Elinor; Cuthbertson, Alan; Desai, Vinay; Pullan, Shirley; Fujii, Dennis K.; Morrison, Matthew; Pither, Richard; Waldman, Scott A.

CORPORATE SOURCE: Research and Development Department, Targeted Diagnostics and Therapeutics, Inc., West Chester, PA, 19380, USA

SOURCE: Journal of Nuclear Medicine (2002), 43(3), 392-399
CODEN: JNMEAQ; ISSN: 0161-5505

PUBLISHER: Society of Nuclear Medicine

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Guanylyl cyclase C (GC-C) is a transmembrane receptor expressed by human intestinal cells and primary and metastatic colorectal adenocarcinomas but not by extraintestinal tissues or tumors. The Escherichia coli heat-stable enterotoxin analog, STa (5-18), is a 14-amino acid peptide that selectively binds to the extracellular domain of GC-C with subnanomolar affinity. This study examined the utility of a radiolabeled conjugate of STa (5-18) to selectively target and image extraintestinal human colon cancer xenografts in vivo in nude mice. The STa conjugate, ethoxyethyl-mercaptoacetamidoadipoylglycylglycine-STa (5-18) (NC100586),

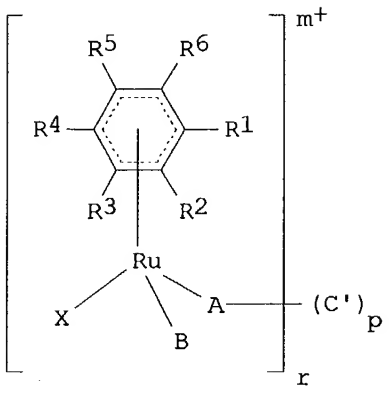
was synthesized and labeled with 99mTc to produce 99mTc-NC100586. This compound was i.v. administered to nude mice bearing human colon cancer xenografts, and specific targeting was evaluated by biodistribution and gamma camera imaging. In CD-1 nude mice, biodistribution and scintigraphic imaging analyses showed selective uptake of 99mTc-NC100586 into human colon cancer xenografts that express GC-C but not into normal tissues that do not express GC-C. Similarly, 99mTc-NC100586 injected i.v. into CD-1 nude mice with human colon cancer hepatic metastases selectively accumulated in those metastases, and .apprx.5-mm foci of tumor cells were visualized after ex vivo imaging of excised livers. Accumulation of 99mTc-NC100586 in human colon cancer xenografts reflected binding to GC-C because 99mTc-NC100588, an inactive analog that does not bind to GC-C, did not selectively accumulate in cancer xenografts compared with normal tissues. Also, coadministration of excess unlabeled STa (5-18) prevented accumulation of 99mTc-NC100586 in human colon cancer xenografts. Furthermore, 99mTc-NC100586 did not selectively accumulate in Lewis lung tumor xenografts, which do not express GC-C. This study showed that i.v. administered STa (5-18) selectively recognizes and binds to GC-C expressed by human colon cancer cells in vivo. Also shown was the ability to exploit this selective interaction to target imaging agents to extraintestinal human colon tumors in nude mice. These results suggest the utility of STa and GC-C for the development of novel targeted imaging and therapeutic agents with high specificity for metastatic colorectal tumors in humans.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:31461 CAPLUS
DOCUMENT NUMBER: 136:85944
TITLE: Half-sandwich ruthenium(II) compounds comprising heteroatom containing ligands for treatment of cancer
INVENTOR(S): Morris, Robert Edward; Sadler, Peter John; Jodrell, Duncan; Chen, Haimei
PATENT ASSIGNEE(S): University Court, the University of Edinburgh, UK
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002002572 | A1 | 20020110 | WO 2001-GB2824 | 20010626 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1294732 | A1 | 20030326 | EP 2001-945472 | 20010626 |
| EP 1294732 | B1 | 20040818 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2001012122 | A | 20030513 | BR 2001-12122 | 20010626 |
| JP 2004502696 | T2 | 20040129 | JP 2002-507824 | 20010626 |
| US 2004029852 | A1 | 20040212 | US 2003-312940 | 20030815 |
| PRIORITY APPLN. INFO.: | | | GB 2000-16052 A | 20000630 |

OTHER SOURCE(S): MARPAT 136:85944
GI




I

AB The preparation of compds. [I; wherein R1 and R2 together with the ring to which they are bound represent a saturated or unsatd. carbocyclic or heterocyclic group; R3, R4, R5, R6, independently = H, alkyl, aryl, alkaryl, or CO2R' (R' = alkyl, aryl, or alkaryl); X = halo, H2O, sulfoxy, carboxy, etc.; A and B, independently = O-donor, N-donor, or S-donor ligands, or halo; C' = (C1-C12)alkylene, optionally substituted in or on the alkylene chain, bound to two A groups; p = 0, 1 and r = 1 when p = 0 and r = 2 when p = 1; m = 0, 1] is described. Thus, 1,4,9,10-tetrahydroanthracene is reacted with RuCl3•3H2O to give 89% [(η6-C14H12)RuCl2]2, which was complexed with ethylenediamine (en) in the presence of NH4PF6 to give 33% [(η6-C14H12)RuCl(en)]+PF6-. Compds. I are useful as antitumor agents, exhibiting IC50 values as high as 315μM against A2780 ovarian cancer cell line. Biol. data are given.
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:936129 CAPLUS
DOCUMENT NUMBER: 136:194211
TITLE: Erythropoietin Mimetics Derived from Solution Phase Combinatorial Libraries
AUTHOR(S): Goldberg, Joel; Jin, Qing; Ambroise, Yves; Satoh, Shigeki; Desharnais, Joel; Capps, Kevin; Boger, Dale L.
CORPORATE SOURCE: Department of Chemistry, The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (2002), 124(4), 544-555
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The erythropoietin receptor (EPOr) is activated by **ligand**-induced homodimerization, which leads to the proliferation and differentiation of erythroid progenitors. Through the screening of combinatorial libraries of dimeric iminodiacetic acid diamides, novel

small mol. binders of EPOr were identified in a protein binding assay. Evaluation of a series of analogs led to optimization of binding subunits, and these were utilized in the synthesis of higher order dimer, trimer, and tetramer libraries. Several of the most active EPOr binders were found to be partial agonists and induced concentration-dependent proliferation of an EPO-dependent cell line (UT-7/EPO) while having no effect on a cell line lacking the EPOr (FDC-P1). An addnl. compound library, based on a sym. isoindoline-5,6-dicarboxylic acid template and including the optimized binding subunits, was synthesized and screened leading to the identification of addnl. EPO mimetics.

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:404409 CAPLUS

DOCUMENT NUMBER: 135:146263

TITLE: Syntheses and structures of two mixed ligands lanthanide complexes with N,N'-substituted adipamide

AUTHOR(S): Xu, Qing-feng; Dai, Jie; Zhao, Bei; Wang, Han-zhang; Zhang, Dao; Yu, Kai-bei

CORPORATE SOURCE: Department of Chemistry, Suzhou University, Suzhou, 215006, Peop. Rep. China

SOURCE: Jiegou Huaxue (2001), 20(3), 168-172
CODEN: JHUADF; ISSN: 0254-5861

PUBLISHER: Jiegou Huaxue Bianji Weiyuanhui

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:146263

AB Neodymium(III) and dysprosium(III) nitrate complexes with the new **ligand** N,N'-dimethyl-N,N'-diphenyladipamide (mpaa), [Nd(mpaa)(DMSO)(NO3)3]2 (1) and Dy(mpaa)2(DMSO)(NO3)3 (2), were prepared and characterized by x-ray crystallog. Both complexes are triclinic with space group P.hivin.1, formula [C22H30N5NdO12S]2 (1) [C42H54N7DyO14S (2)], Mr = 1465.62[1075.48], a = 8.541(1)[9.711(2)], b = 11.915(1)[16.017(3)], c 15.906(1)[16.686(3)] Å, α 107.22(1)[109.600(1)], β = 98.12(1)[92.50(1)], γ 99.78(1)°[96.22(1)]°, V = 1491.8(2)[2421.7(8)] Å3, dc = 1.631[1.475] g·cm-3, Z = 1[2], F(000) = 738[1098], μ = 0.71073 cm-1; R = 0.0261[0.0364], Rw = 0.0611[0.0857] reflections with 1>2 σ (I). Complex 1 is dinuclear, in which two Nd(III) ions are double-bridged by two mpaa ligands. And 2 is a mononuclear complex, in which one of the two C:O groups in MPAA is uncoordinated. In the two above complexes, each Ln(III) ion is nine-coordinated including three bidentate nitrates, one DMSO mol. and two carbonyl oxygens from two different mpaa ligands. Neutral monodentate DMSO enters the coordination sphere to meet the geometric requirements. When the number of methylene between O:C···C:O in diamides (R1R2NCO)2(CH2)n was increased, the **ligand** prefers to act as a bridging reagent rather than a chelate.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:318507 CAPLUS

DOCUMENT NUMBER: 135:91483

TITLE: A structure-function study of **ligand** recognition by CD22β

AUTHOR(S): Van Rossenberg, Sabine M. W.; Sliedregt, Leo A. J. M.; Autar, Reshma; Piperi, Christina; Van der Merwe, Anton P.; Van Berkel, Theo J. C.; Kuiper, Johan; Biessen, Erik A. L.

CORPORATE SOURCE: Leiden / Amsterdam Center for Drug Research, Division

of Biopharmaceutics, Sylvius Laboratories, Leiden University, Leiden, 2300 RA, Neth.
SOURCE: Journal of Biological Chemistry (2001), 276(16), 12967-12973
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB B-cell-specific CD22 is a member of a group of cell adhesion mols. within the Ig superfamily that display binding to glycans with terminal sialic acid residues. Binding of endogenous ligands to CD22 triggers B-cell activation and proliferation. It is therefore conceivable that high affinity ligands for CD22 may be of value as inhibitors of B-cell activation in allergy and chronic inflammation. In this study, we aimed to delineate the structural requirements for **ligand** binding to CD22. A library of 20 mono-, di-, and trisaccharide analogs of the basic binding motif Neu5Ac(α2,6)Lac was synthesized and screened for affinity for CD22β. In general, CD22 **ligand** recognition appeared to be rather tolerant with respect to structural modifications of the anomeric sugar on a mono-, di-, and trisaccharide level, although affinity was increased by the presence of a nitro aromatic group at C-2. The most potent monovalent **ligand**, Neu5Ac-4-nitrobenzoyl-Glc, was selected to generate multivalent ligands based on either a glutamate or Tris cluster core. All multivalent ligands displayed at least a 10-fold increased affinity for CD22 compared with the corresponding monovalent glycoside. Interestingly, a maximal gain in affinity was already obtained for bivalent ligands, regardless of the terminal glycoside. A trivalent Tris-based cluster of Neu5Ac-4-nitrobenzoyl-Glc displayed a 300-fold higher affinity compared with the basic binding motif, which makes it, to our knowledge, the most potent antagonist for CD22 yet synthesized. As our in vitro fluorescence-activated cell sorting studies demonstrated efficient cellular uptake of a CD22 substrate, the most potent **ligand** in this study may hold promise as a homing device for immunomodulatory compds. and cytostatics.
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:168124 CAPLUS
DOCUMENT NUMBER: 134:218936
TITLE: Crystal structure of CDC25 proteins and its use in rational design of inhibitors
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001016300 | A2 | 20010308 | WO 2000-US23473 | 20000825 |
| WO 2001016300 | A3 | 20020530 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1226237 A2 20020731 EP 2000-959449 20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

PRIORITY APPLN. INFO.: US 1999-172215P P 19990831
WO 2000-US23473 W 20000825

OTHER SOURCE(S): MARPAT 134:218936

AB The present invention relates to polypeptides which comprise the **ligand** binding domain of CDC25, crystalline forms of these polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of CDC25 alone and in complexes with pentapeptide inhibitors. Atomic coordinates are provided from x-ray diffraction of crystals of CDC25A and CDC25B catalytic domains in the presence and absence of various inhibitors. The invention also relates to the use of the 3-dimensional structure of the CDC25 catalytic domain in methods of designing and/or identifying potential inhibitors of CDC25 activity, for example, compds. which inhibit the binding of a native substrate to the CDC25 catalytic domain. The method comprises the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the CDC25 catalytic domain, and (2) identifying a scaffold which presents the functional group or functional groups in a suitable orientation for interacting with one or more subsites of the CDC25 catalytic domain. Since CDC25 is a potential target for therapies aimed at controlling proliferative disease, the atomic coordinates allow rational structure-based design of potential agents for the treatment of cancer, restenosis, reocclusion of coronary artery, or inflammation.

L4 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:281605 CAPLUS
DOCUMENT NUMBER: 133:147140
TITLE: Estimation of Receptor-**Ligand** Interactions by the Use of a Two-Marker System in Affinity Capillary Electrophoresis
AUTHOR(S): Mito, Erica; Zhang, Ying; Esquivel, Sally; Gomez, Frank A.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, California State University, Los Angeles, CA, 90032, USA
SOURCE: Analytical Biochemistry (2000), 280(2), 209-215
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The study of receptor-**ligand** interactions by affinity capillary electrophoresis (ACE) requires an accurate form of anal. Here, we examine the use of two noninteracting stds. (markers) in the anal. of binding constant data in ACE studies. This concept is demonstrated using two model systems: carbonic anhydrase B (CAB, EC 4.2.1.1) and arylsulfonamides, and vancomycin (Van) from Streptomyces orientalis and the dipeptide N-acetyl-d-Ala-d-Ala. In this procedure a plug of receptor and noninteracting stds. is injected, and anal. of the change in the relative migration time ratio of the receptor, relative to the noninteracting stds., as a function of the concentration of the **ligand** yields a value for the binding constant The findings described here demonstrate that data

from ACE studies can best be analyzed using two noninteracting stds., yielding values comparable to those estimated using other binding and ACE techniques. (c) 2000 Academic Press.
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:186322 CAPLUS
DOCUMENT NUMBER: 132:342333
TITLE: [RuII(hedta)]- complexes of 2,2'-dipyridylamine (dpaH) and a bifunctional tethered analog, N,N,N',N'-tetrakis(2-pyridyl)adipamide (tpada)
AUTHOR(S): Shepherd, R. E.; Chen, Y.; Kortes, R. A.; Ward, M. S.
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, USA
SOURCE: Inorganica Chimica Acta (2000), 303(1), 30-39
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [RuII(hedta)(dpaH)]- [hedta3- = N-(hydroxyethyl)ethylenediamine-N,N,N'-triacetate, dpaH = 2,2'-dipyridylamine] and [{RuII(hedta)}2(μ-tpada)] [tpda = N,N,N',N'-tetrakis(2-pyridyl)adipamide] were studied by 1H NMR and electrochem. methods in aqueous solution The bidentate rings of dpaH and tpada are differentiated as shown by NMR upon coordination to RuII due to differences in the local environment. The dpa-R headgroup of each **ligand** binds 'in-plane' with the en backbone of hedta3- and with one pyridyl ring being nearer the amine of hedta3- having the pendant glycinato group [matching the known arrangement with bpy (2,2'-bipyridine)]. RuII/III E1/2 values follow the order dpaH (0.32 V) < tpada (0.47 V) < bpy (0.54 V), showing that dpaH is a weaker π-acceptor **ligand** than bpy, and that the withdrawing carbonyl functionality enhances the π-acceptor capacity for the tpada **ligand,** approaching the stability imparted by bpy. Only the 1:1 [RuII(hedta)(dpaH)]- complex forms even in the presence of excess dpaH. [RuII(hedta)(dpaH)] has a pKa of the dipyridylamine proton of .apprx.5.0 with [RuIII(hedta)(dpa-)] undergoing aquation (kH2O = 1.4 + 10-2 s-1) and OH--assisted dissociation (kOH = 1.33 + 104 M-1 s-1). The {[RuII(hedta)]2(tpada)}2- complex serves as a water-soluble model as to how {[ML']2(tpada)} complexes might act as an extended bridge between two metal binding sites, potentially those of metallo-derivatized DNA strands, or between one DNA strand and a protein crosslink. In this model M represents an appropriate metal for DNA derivatization such as RuII, PtII or PdII and L' represents the attachments to DNA nucleobase sites, aminocarboxylates/peptide coordination for antitumor purposes.
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:534605 CAPLUS
DOCUMENT NUMBER: 131:333744
TITLE: A surface-modified functional liposome capable of binding to cell membranes
AUTHOR(S): Yagi, Nobuhiro; Ogawa, Yoshikatsu; Kodaka, Masato; Okada, Tomoko; Tomohiro, Takenori; Okuno, Hiroaki; Yagi, Nobuhiro; Konakahara, Takeo
CORPORATE SOURCE: Biomolecules Department, National Institute of Bioscience and Human-Technology, Tsukuba, Ibaraki, 305-8566, Japan
SOURCE: Chemical Communications (Cambridge) (1999), (17), 1687-1688
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A liposome including the lipopeptide RGD-C4A2, whose surface is modified by a GRGDS-repeating peptide **ligand**, is found to bind to NIH3T3 cells via the interaction between the peptide **ligand** and the membrane receptor.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:443257 CAPLUS
DOCUMENT NUMBER: 132:93620
TITLE: Synthesis of a novel lipopeptide with α-melanocyte-stimulating hormone peptide **ligand** and its effect on liposome stability. [Erratum to document cited in CA131:88183]
AUTHOR(S): Ogawa, Yoshikatsu; Kawahara, Hidehiko; Yagi, Nobuhiro; Kodaka, Masato; Tomohiro, Takenori; Okada, Tomoko; Konakahara, Takeo; Okuno, Hiroaki
CORPORATE SOURCE: Biomolecules Dep., National Institute Bioscience and Human-Technology, Ibaraaki, 305-8566, Japan
SOURCE: Lipids (1999), 34(6), 643
CODEN: LPDSAP; ISSN: 0024-4201
PUBLISHER: AOCS Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A corrected structure is given for Scheme 2.

L4 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:425527 CAPLUS
DOCUMENT NUMBER: 131:87829
TITLE: Preparation of N-(4-amino-6-quinolyl)carboxamides as chemokine receptor ligands and as anti-AIDS drugs
INVENTOR(S): Hagmann, William K.; Springer, Martin S.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 19 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5919776 | A | 19990706 | US 1997-993494 | 19971218 |
| PRIORITY APPLN. INFO.: | | | US 1997-993494 | 19971218 |

OTHER SOURCE(S): MARPAT 131:87829
AB R3R2NZR4 [R2,R3 = H, (ar)alkyl, aryl, etc.; NR2R3 = heterocyclyl; R4 = NHCOXR7, CONHR7, NR8R9, etc.; R7 = H, alkyl, (hetero)aryl(alkyl), etc.; R8,R9 = H, alkyl, Ph; X = bond, O, NR8; Z = 2-(un)substituted quinoline-4,6-diyl] were prepared as chemokine receptor ligands and as anti-AIDS drugs (no data). Thus, 4,6-diamino-2-methylquinoline was amidated by (COCl)2 to give (H2NZNHCO)2 (Z = 2-aminoquinoline-4,6-diyl).
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:397363 CAPLUS
DOCUMENT NUMBER: 131:182178
TITLE: Binding of a dimeric derivative of vancomycin to L-Lys-D-Ala-D-lactate in solution and at a surface

AUTHOR(S): Rao, Jianghong; Yan, Lin; Lahiri, Joydeep; Whitesides, George M.; Weis, Robert M.; Warren, H. Shaw

CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SOURCE: Chemistry & Biology (1999), 6(6), 353-359
CODEN: CBOLE2; ISSN: 1074-5521

PUBLISHER: Current Biology Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The emergence of bacteria that are resistant to vancomycin (V), a glycopeptide antibiotic, results from the replacement of the carboxy-terminal D-Ala-D-Ala of bacterial cell wall precursors by D-Ala-D-lactate. Recently, it has been demonstrated that covalent dimeric variants of V are active against vancomycin-resistant enterococci (VRE). To study the contribution of divalency to the activities of these variants, we modeled the interactions of V and a dimeric V with L-Lys-D-Ala-D-lactate, an analog of the cell-wall precursors of the vancomycin-resistant bacteria. A dimeric derivative of V (V-Rd-V) was found to be much more effective than V in inhibiting the growth of VRE. The interactions of V and V-Rd-V with a monomeric lactate **ligand** - diacetyl-L-Lys-D-Ala-D-lactate (Ac2KDADLac) - and a dimeric derivative of L-Lys-D-Ala-D-lactate (Lac-R'd-Lac) in solution have been examined using isothermal titration calorimetry and UV spectroscopy titrns.; the results reveal that V-Rd-V binds Lac-R'd-Lac approx. 40 times more tightly than V binds Ac2KDADLac. Binding of V and of V-Rd-V to Nα-Ac-L-Lys-D-Ala-D-lactate presented on the surface of mixed self-assembled monolayers (SAMs) of alkanethiolates on gold indicates that the apparent off-rate for dissociation of V-Rd-V from the surface is much slower than that of V from the same surface. The results are compatible with the hypothesis that divalency is responsible for tight binding, which correlates with small values of min. inhibitory concns. of V and V-Rd-V.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:321129 CAPLUS

DOCUMENT NUMBER: 131:88183

TITLE: Synthesis of a novel lipopeptide with α-melanocyte-stimulating hormone peptide **ligand** and its effect on liposome stability

AUTHOR(S): Ogawa, Yoshikatsu; Kawahara, Hidehiko; Yagi, Nobuhiro; Kodaka, Masato; Tomohiro, Takenori; Okada, Tomoko; Konakahara, Takeo; Okuno, Hiroaki

CORPORATE SOURCE: Biomolecules Department, National Institute of Bioscience and Human-Technology, Ibaraki, 305-8566, Japan

SOURCE: Lipids (1999), 34(4), 387-394
CODEN: LPDSAP; ISSN: 0024-4201

PUBLISHER: AOCS Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Introduction of liposomes into target cells is important for drug delivery systems. For this purpose, the surface of the liposome is equipped with **ligand** peptides, which may bind to specific receptors on the cell membrane. An artificial novel lipopeptide (MSH-C4A2) containing the α-MSH sequence and two long alkyl chains was designed and synthesized, and the liposome, composed of egg phosphatidylcholine (EPC) and MSH-C4A2, was prepared The stability of the liposome was estimated by measuring calcein leakage from the liposome inner phase. The stability of the liposome decreased upon addition of MSH-A4C2, which seemed to be attributable to the amphiphilic property of the peptide moiety (α-MSH) of MSH-A2C4. The stability was, however, recovered fairly

well upon addition of cholesterol (Ch) or phosphatidylglycerol (PG). It was concluded therefore that the ternary system, MSH-C4A2/Ch/EPC or MSH-C4A2/PG/EPC, is suitable for preparing the functional liposome.
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:261683 CAPLUS
DOCUMENT NUMBER: 131:55769
TITLE: Synthesis and characterization of model compounds of the active site of the enzyme superoxide dismutase
AUTHOR(S): Morales, Jose Luis Garate; Vergara, Enrique Gonzalez
CORPORATE SOURCE: Centro de Quimica Instituto de Ciencias. BUAP, Puebla de Zaragoza, Mex.
SOURCE: Congreso Iberoamericano de Quimica Inorganica, 6th, Puebla, Mex., Apr. 20-25, 1997 (1997), 47-50. Asociacion Mexicana de Quimica Inorganica: Guanajuato, Mex.
CODEN: 67NIAA
DOCUMENT TYPE: Conference
LANGUAGE: Spanish
AB Five Cu(II) complexes with bi-, tri- or tetradentate ligands containing imidazole N as donor atom were synthesized for spectrophotometric modeling of the active site of superoxide dismutase. Characterization of these complex by UV and IR spectroscopy indicated that they displayed some characteristics of the enzyme. The Cu(II)-PEDTA20 complex reproduced the visible spectrum of superoxide dismutase. However, the EPR data corresponded better to the characteristics of other Cu(II) enzymes, so the initial objective was modified to spectroscopic modeling of other Cu metalloproteins.
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:238153 CAPLUS
DOCUMENT NUMBER: 131:19206
TITLE: Synthesis of neoglycoconjugate dendrimers
AUTHOR(S): Tsvetkov, Dmitry E.; Cheshev, Pavel E.; Tuzikov, Alexander B.; Pazynina, Galina V.; Bovin, Nikolai V.; Rieben, Robert; Nifant'ev, Nikolay E.
CORPORATE SOURCE: N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 117913, Russia
SOURCE: Mendeleev Communications (1999), (2), 47-50
CODEN: MENCEX; ISSN: 0959-9436
PUBLISHER: Russian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of polydentate dendritic neoglycoconjugates which contain 4, 8, 16, 32 B-disaccharide ligands were designed as probes to assess the influence of inter-**ligand** distance on binding to anti-B-disaccharide Igs.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:163629 CAPLUS
DOCUMENT NUMBER: 131:180
TITLE: Cytotoxicity of (2,2':6',2''-Terpyridine)platinum(II) Complexes to Leishmania donovani, Trypanosoma cruzi, and Trypanosoma brucei
AUTHOR(S): Lowe, Gordon; Droz, Anne Sophie; Vilaivan, Tirayut; Weaver, George W.; Tweedale, Lindsay; Pratt, Jonathan

M.; Rock, Peter; Yardley, Vanessa; Croft, Simon L.
CORPORATE SOURCE: Dyson Perrins Laboratory, Oxford University, Oxford, OX1 3QY, UK
SOURCE: Journal of Medicinal Chemistry (1999), 42(6), 999-1006
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A range of (2,2':6',2''-terpyridine)platinum(II) complexes are shown to possess antiprotozoal activity in vitro against Leishmania donovani, Trypanosoma cruzi, and Trypanosoma brucei, the causative organisms of tropical diseases leishmaniasis and trypanosomiasis. The best compds. caused 100% and 78% inhibition of growth of the intracellular amastigote forms of L. donovani and T. cruzi, resp., at a concentration of 1 μM and 100% inhibition of growth of the bloodstream trypomastigote forms of T. brucei at a concentration of 0.03 μM. The results obtained with complexes in which the fourth **ligand** to platinum(II) is capable of being substituted with a substitution inert hydroxyethanethiolate complex are compared. The ammine complexes show high antiprotozoal activity suggesting that the trans influence of the 2,2':6',2''-terpyridine **ligand** has a profound effect on the ease of displacement of the fourth **ligand** in (2,2':6',2''-terpyridine)platinum(II) complexes, although nonbonded interaction between the ammine **ligand** and the 6 and 6'' hydrogens probably also weakens the ligation to Pt(II).
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:437199 CAPLUS
DOCUMENT NUMBER: 129:213752
TITLE: The use of affinity capillary electrophoresis for determining binding constants of ligands to receptors
AUTHOR(S): Zhao, Dong S.; Kwak, Eun-Soo; Kawaoka, Jane; Esquivel, Sally; Gomez, Frank A.
CORPORATE SOURCE: Univ. California, Riverside, CA, USA
SOURCE: American Laboratory (Shelton, Connecticut) (1998), 30(12), 40, 42-47
CODEN: ALBYBL; ISSN: 0044-7749
PUBLISHER: International Scientific Communications, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The paper reports on using affinity capillary electrophoresis (ACE) to determine binding consts. between three receptor -**ligand** combinations: carbonic anhydrase B and arylsulfonamides; vancomycin and the peptide N-acetyl-D-Ala-D-ALa; adamantane carboxylic acids and β-cyclodextrin derivs.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:350876 CAPLUS
DOCUMENT NUMBER: 129:81953
TITLE: Modification of receptor selectivity and functional activity of cyclic cholecystokinin analogs
AUTHOR(S): Amblard, Muriel; Rodriguez, Marc; Lignon, Marie-Francoise; Galas, Marie-Christine; Bernad, Nicole; Aumelas, Andre; Martinez, Jean
CORPORATE SOURCE: Faculte de Pharmacie, CNRS - UMR 5810, Montpellier I et II, Montpellier, 34060, Fr.
SOURCE: European Journal of Medicinal Chemistry (1998), 33(3), 171-180

CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors reported earlier on the synthesis and biol. activity at the cholecystokinin-B (CCK-B) receptor of cyclized CCK derivs. These peptides, in which the positions 28 and 31 were replaced by Lys residues, were bridged by a succinyl moiety. To determine the importance of the nature and size of the cyclic structure, cyclic analogs were synthesized in which: (i) the Lys residues were replaced by ornithine and diaminobutyric acid and (ii) the succinic moiety was replaced by a malonic, adipic and glutaric moiety. They were tested for their ability to inhibit the specific binding of 125I-BH-CCK-8 to CCK receptors in rat pancreatic acini and guinea pig brain membranes. They were also evaluated for their ability to stimulate amylase secretion from rat pancreatic acini. The potency and selectivity of these analogs were compared with those obtained with CCK-4 and compound JMV320, a potent and selective CCK-B receptor **ligand** synthesized earlier in the authors' laboratory

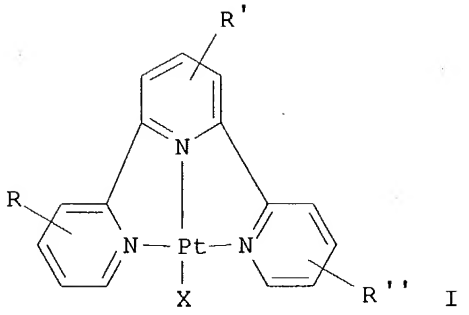
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:513635 CAPLUS
DOCUMENT NUMBER: 127:199246
TITLE: Preparation of terpyridine-platinum(II) complexes as potent intercalators of DNA, and as antitumor and antiparasitic agents
INVENTOR(S): Lowe, Gordon
PATENT ASSIGNEE(S): Isis Innovation Ltd., UK; Lowe, Gordon
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9727202 | A1 | 19970731 | WO 1997-GB218 | 19970124 |
| W: CA, JP, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| CA 2241992 | AA | 19970731 | CA 1997-2241992 | 19970124 |
| EP 885233 | A1 | 19981223 | EP 1997-901187 | 19970124 |
| EP 885233 | B1 | 20020619 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE, IE, FI | | | | |
| JP 2000503982 | T2 | 20000404 | JP 1997-526675 | 19970124 |
| EP 1164138 | A1 | 20011219 | EP 2001-121776 | 19970124 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE, IE, FI | | | | |
| AT 219493 | E | 20020715 | AT 1997-901187 | 19970124 |
| ES 2175330 | T3 | 20021116 | ES 1997-901187 | 19970124 |
| US 2002013306 | A1 | 20020131 | US 1998-101556 | 19980713 |

PRIORITY APPLN. INFO.: GB 1996-1603 A 19960126
EP 1997-901187 A3 19970124
WO 1997-GB218 W 19970124

OTHER SOURCE(S): MARPAT 127:199246
GI

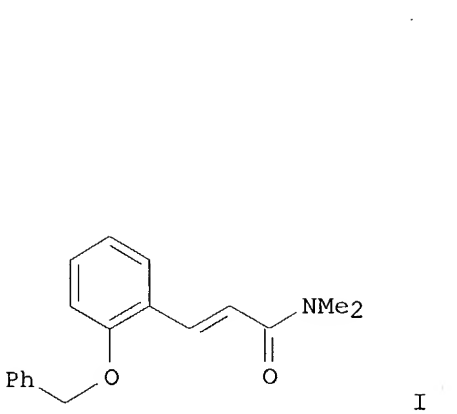


I

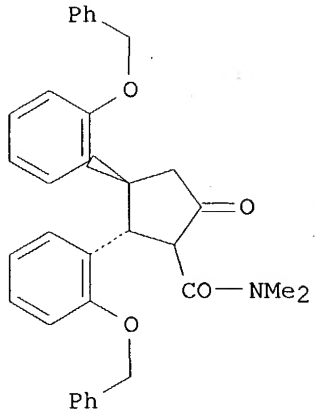
AB A new class of (un)substituted 2,2':6',2''-terpyridine-Pt(II) complexes I, in which an N- or O- or halo nucleophile is the fourth **ligand** to Pt, are prepared by a new method which involves reacting a Pt complex of 1,5-cyclooctadiene (or other strong bis-trans-labilizing **ligand**) with a 2,2':6',2''-terpyridine in the presence of MeCN. Compds. I and their water-soluble salts include X = aromatic heterocycle or Rn3, substituted aromatic heterocycle linked to Pt through N, or a nitrile (R4CN), an amine (R5NH2), an alc. (R6OH), NH3, or water linked to Pt through the resp. N or O, or halo. R, R' and R'' are the same or different and include H, alkyl, aryl, aralkyl, alkaryl, acyl, halo, haloalkyl, haloaryl, hydroxyalkyl, hydroxyaryl, aminoalkyl, aminoaryl, primary, secondary or tertiary amine, hydrazine, alkylhydrazine, alkoxy, aralkoxy, nitrile, ester, amide, nitro, azide, aziridino, or is a covalently linked chain which forms a dimeric or oligomeric species. R3 is a pos. charged group or is defined as R, R' or R'', and n = 1, 2 or 3 provided that when each R, R' and R'' is H, then X ≠ Cl. The compds. are potent intercalators of DNA. Some compds. I have antitumor activity. The most effective compds. have antitumor activity comparable to or better than cisplatin and show little or no cross resistance. Such compds. are more effective than cisplatin against cisplatin-resistant cell lines. Other compds. are most effective against doxorubicin resistant cell lines. Some compds. I have antiparasitic activity. In vitro antiprotozoal activities against Leishmania donovani, Trypanosoma cruzi, Trypanosoma brucei, and Plasmodium falciparum are demonstrated. Ribonucleoside or 2'-deoxyribonucleosides base-labeled with the 2,2':6',2''-terpyridine-Pt(II) complexes are prepared and are of use to disrupt DNA replication.

L4 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

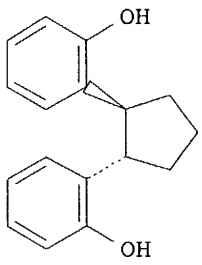
ACCESSION NUMBER: 1996:725712 CAPLUS
DOCUMENT NUMBER: 126:103882
TITLE: dl-Selective reductive coupling/Dieckmann condensation sequence of α,β-unsaturated amides with samarium(II) iodide/HMPA. Synthesis of a new **ligand**, trans-1,2-cyclopentanediyl-2,2'-bis(phenol)
AUTHOR(S): Kanemasa, Shuji; Yamamoto, Hidetoshi; Kobayashi, Shigeru
CORPORATE SOURCE: Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan
SOURCE: Tetrahedron Letters (1996), 37(47), 8505-8506
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI




I




II




III

AB By action of SmI2-HMPA in THF, (E)-N,N-dimethyl-α,β-unsatd. amides gave 1,2-trans-2,3-trans stereoisomers of 2,3-disubstituted 5-oxo-1-cyclopentanecarboxamides via a highly dl-selective reductive coupling followed by Dieckmann condensation. Water-d2 was an effective quenching agent. This reaction was applied to the preparation of trans-1,2-cyclopentanediyl-2,2'-biphenol, which is a new C2-sym. chiral **ligand**. The reaction of (E)-N,N-dimethyl-3-[(2-phenylmethoxy)phenyl]-2-propenamide (I) with samarium iodide gave II. Subsequent hydrolysis and reduction of II gave trans-2,2'-(1,2-cyclopentanediyl)bis[phenol] (III).

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:851985 CAPLUS

DOCUMENT NUMBER: 124:185539

TITLE: Nanoparticles containing an active agent and a poly(tartaramide ketal)

INVENTOR(S): Ahlers, Michael; Walch, Axel; Seipke, Gerhard; Russell-Jones, Gregory

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 671169 | A1 | 19950913 | EP 1995-103045 | 19950303 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| DE 4407898 | A1 | 19950914 | DE 1994-4407898 | 19940309 |

| | | | | | |
|---|---|---|---|---|---|
| TW 457096 | B | 20011001 | TW 1995-84101519 | | 19950220 |
| FI 9501053 | A | 19950910 | FI 1995-1053 | | 19950307 |
| US 5674531 | A | 19971007 | US 1995-399474 | | 19950307 |
| IL 112905 | A1 | 20000831 | IL 1995-112905 | | 19950307 |
| CA 2144216 | AA | 19950910 | CA 1995-2144216 | | 19950308 |
| NO 9500889 | A | 19950911 | NO 1995-889 | | 19950308 |
| AU 9514701 | A1 | 19950921 | AU 1995-14701 | | 19950308 |
| AU 685577 | B2 | 19980122 | | | |
| JP 07258114 | A2 | 19951009 | JP 1995-48006 | | 19950308 |
| ZA 9501910 | A | 19951113 | ZA 1995-1910 | | 19950308 |
| HU 72033 | A2 | 19960328 | HU 1995-698 | | 19950308 |
| PRIORITY APPLN. INFO.: | | | DE 1994-4407898 | A | 19940309 |

GI For diagram(s), see printed CA Issue.

AB Nanoparticles of poly(tartaramide ketal) [I; R2 = (substituted) alkylene, cycloalkylene] are useful as biocompatible, biodegradable carriers for drugs, especially peptides and proteins. The nanoparticles may be functionalized with specific ligands which facilitate receptor-mediated transport through the intestinal wall. Thus; DL-tartaric acid was refluxed in MeOH with 2,2-dimethoxypropane and p-toluenesulfonic acid to form di-Me 2,3-O-isopropylidene-DL-tartrate, which was polymerized with 1,8-diaminooctane. A solution of this polymer 280, polylysine 60, and insulin 40 mg in MeOH was spray dried to produce nanoparticles 330 nm in diameter

L4 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:702992 CAPLUS

DOCUMENT NUMBER: 123:186764

TITLE: Synthesis, characterization and biological activity of metal complexes of N,N'-bis(8-hydroxy-5-quinolinyl)adipamide

AUTHOR(S): Patel, R. D.

CORPORATE SOURCE: Chemistry Department, Sardar Patel University, Vallabh Vidyanagar, 388120, India

SOURCE: Journal of Indian Council of Chemists (1993), 9(2), 48-51
CODEN: JICCE7; ISSN: 0971-5037

PUBLISHER: Indian Council of Chemists

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complexes prepared from a novel bis-bidentate **ligand** N,N'-bis(8-hydroxy-5-quinolinyl)adipamide with some bivalent metal ions such as Co, Ni, Cu and Zn, were characterized with the aid of anal., magnetic and thermal data along with IR and electronic spectra. All the complexes showed a 1:1 metal to **ligand** stoichiometry and a polymeric nature with an octahedral stereochem. at the coordinated metal atom. The coordination polymers are potentially antifungal exhibiting the activity in the range 40-70%.

L4 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:293370 CAPLUS

DOCUMENT NUMBER: 120:293370

TITLE: Determination of Binding Constants of Ligands to Proteins by Affinity Capillary Electrophoresis: Compensation for Electroosmotic Flow

AUTHOR(S): Gomez, Frank A.; Avila, Luis Z.; Chu, Yen-Ho; Whitesides, George M.

CORPORATE SOURCE: Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA

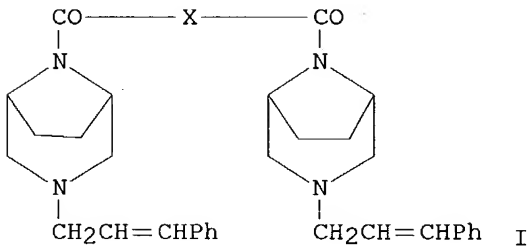
SOURCE: Analytical Chemistry (1994), 66(11), 1785-91
CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper describes the estimation of binding consts. (Kb) between carbonic anhydrase B (CAB, E.C.4.2.1.1, from bovine erythrocytes) and charged benzenesulfonamides by affinity capillary electrophoresis (ACE) under conditions in which the migration time is affected by changes in electroosmotic flow and by nonspecific interactions accompanying changes in the concentration of **ligand**. Comparisons of values of migration times of the protein of interest, and of noninteracting marker proteins, with those of a neutral internal standard provide the basis for corrections for variable electroosmotic flow; these corrections make possible the estimation of Kb and its uncertainty even in the presence of substantial variations in electroosmotic flow.

L4 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:551940 CAPLUS
DOCUMENT NUMBER: 119:151940
TITLE: Synthesis and opioid receptor affinity of bivalent ligands derived from 3,8-diazabicyclo(3.2.1)octanes
AUTHOR(S): Barlocco, Daniela; Fadda, Paola; Fratta, Walter
CORPORATE SOURCE: Ist. Chim. Farm. Toss., Univ. Milano, Milan, 20131, Italy
SOURCE: Farmaco (1993), 48(3), 387-96
CODEN: FRMCE8; ISSN: 0014-827X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

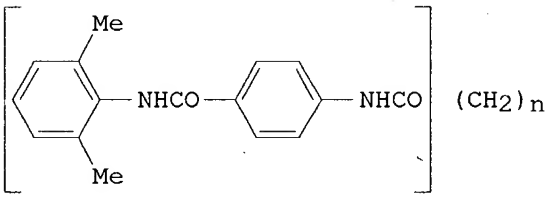
AB A new series of bivalent ligands [I, X = (CH2)2, (CH2)3, (CH2)4 or trans CH2-CH=CH-CH2], derived from the previously reported analgesic 3-cinnamyl-8-propionyl-3,8-diazabicyclo(3.2.1)octaine (II), has been synthesized and tested in vitro for their affinity towards opioid receptors and in vivo for their analgesic potency. None of the new compds. showed either appreciable affinity for opioid receptors or analgesic activity comparable to that of the model II.

opioid

L4 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:465899 CAPLUS
DOCUMENT NUMBER: 117:65899
TITLE: Use of affinity capillary electrophoresis to measure binding constants of ligands to proteins
AUTHOR(S): Chu, Yen Ho; Avila, Luis Z.; Biebuyck, Hans A.; Whitesides, George M.
CORPORATE SOURCE: Dep. Chem., Harvard Univ., Chambridge, MA, 02138, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(15), 2915-17
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In open tubular capillary electrophoresis of carbonic anhydrase B (CAB,

E.C.4.2.1.1, from bovine erythrocytes), addition to the electrophoresis buffer of benzene sulfonamides substituted in the 4-position with neg. charged groups increases the mobility of CAB. Adding NADP+ and NADPH to the electrophoresis buffer also increases the mobility of glucose-6-phosphate dehydrogenase (E.C.1.1.1.49, from Leuconostoc mesenteroides). For calmodulin (bovine testes), increasing concentration of calcium ion in the electrophoresis buffer decreases the mobility of the protein. Analyses of electrophoretic mobilities as a function of the concentration of these ligands yields values for their binding consts. to the corresponding proteins. These values agree well with those estimated using conventional assays. Affinity capillary electrophoresis has the potential to be a sensitive and convenient new method for measuring binding consts. to proteins.

L4 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:135903 CAPLUS
DOCUMENT NUMBER: 114:135903
TITLE: Synthesis and pharmacological evaluation of the anticonvulsant activity of bivalent ligands derived from 4-amino-2',6'-dimethylbenzanilide
AUTHOR(S): Poupaert, J. H.; Hermans, E.; Jonckheere, Y.; Mergen, F.; Lambert, D.; Lerot, T.; Aandrianjara, R.; Poupaert, E. J.; Lybrand, T.; Durant, F.
CORPORATE SOURCE: Sch. Pharm., Cathol. Univ. Louvain, Brussels, B-1200, Belg.
SOURCE: Asia Pacific Journal of Pharmacology (1990), 5(3), 249-51
CODEN: APJPEV; ISSN: 0217-9687
DOCUMENT TYPE: Journal
LANGUAGE: English
GI




I

anticonvulsant
dimethylbenzanilide

AB A homologous series of bivalent ligands (I, n = 1-8) consisting of 2 4-amino-2',6'-dimethylbenzanilide mol.s linked by a ω,ω'-diacylpolymethylene connector of varying length was synthesized and evaluated for anticonvulsant activity. The choice of the 4-amino-2',6'-dimethylbenzanilide moiety was based on its chemical simplicity, its high potency and selectivity and its intrinsic rigidity as illustrated by energy refinement and mol. dynamics studies based on x-ray data. The compds. were tested in mice by the maximum electroshock seizure test. Only I (n = 3) showed a modest activity indicating that probably no bridging of proximal receptor sites occurs.

L4 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:191480 CAPLUS
DOCUMENT NUMBER: 112:191480
TITLE: Molecular recognition between oligopeptides and nucleic acids: DNA binding specificity of a series of bis netropsin analogs deduced from footprinting analysis
AUTHOR(S): Kissinger, Koren L.; Dabrowiak, James C.; Lown, J.

William
CORPORATE SOURCE: Dep. Chem., Syracuse Univ., Syracuse, NY, 13244-1200, USA
SOURCE: Chemical Research in Toxicology (1990), 3(2), 162-8
CODEN: CRTOEC; ISSN: 0893-228X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:191480

AB A series of tether-linked bisnetropsins were prepared in order to assess the phasing problem, which arises because of the lack of dimensional correspondence between oligopeptides and oligonucleotides in DNA binding characteristics. The consequences of incorporating variable-length flexible and rigid tethers [poly(methylene), Z and E ethylene, m- and p-phenylene] between the 2 netropsin-like moieties on the DNA binding properties were assessed by DNase I footprinting. The conformational freedom associated with 2 netropsins linked by a flexible methylene tether allows **ligand** binding in both a mono- and bidentate fashion, with bidentate binding requiring a min. linker length of (CH2)6. For compds. possessing rigid tethers, for example, cis and trans ethylene moieties, the cis geometry excludes bidentate ligation, while the trans structure favors it. Bisnetropsins possessing aryl linking groups have reduced DNA binding affinities. This is most plausibly due to the aryl groups, which are not coplanar with the netropsin moieties, thus blocking the **ligand** from penetrating deeply into the minor groove of DNA.

=> FIL STNGUIDE

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 107.50 | 280.49 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -21.70 | -23.10 |

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|---|---|---|
| FULL ESTIMATED COST | 0.30 | 280.79 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -23.10 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:25:13 ON 23 SEP 2004